

The leading asymptotic terms of the three-body Coulomb scattering wave function

A. M. Mukhamedzhanov,¹ A. S. Kadyrov,² and F. Pirlepesov¹

¹*Cyclotron Institute, Texas A&M University, College Station, TX 77843, USA*

²*Centre for Atomic, Molecular and Surface Physics,*

Division of Science and Engineering, Murdoch University, Perth 6150, Australia

(Dated: February 4, 2008)

The asymptotic wave function derived by Alt and Mukhamedzhanov [Phys. Rev. A 47, 2004 (1993)] and Mukhamedzhanov and Lieber [Phys. Rev. A 54, 3078 (1996)] has been refined in the region where the pair (β, γ) remains close to each other while the third particle α is far away from them ($\rho_\alpha \rightarrow \infty$, $r_\alpha/\rho_\alpha \rightarrow 0$). The improved wave function satisfies the Schrödinger equation up to the terms of order $O(1/\rho_\alpha^3)$, provides the leading asymptotic terms of the three-body scattering wave function with Coulomb interactions and gives further insight into the continuum behavior of the three-charged-particle wave function and helps to obtain $3 \rightarrow 3$ scattered wave. This opens up further ways of solving and analysing the three-body Schrödinger equation by numerical means.

PACS numbers: 21.45.+v, 25.10.+s, 03.65.Nk, 34.10.+x

I. INTRODUCTION

The quantum dynamics of three charged particles is described by Schrödinger's equation which should be supplemented by proper boundary conditions. Merkuriev and Faddeev [1] claimed that the solution of this equation exists and is unique if the boundary conditions are known in all asymptotic regions. There are two types of the three-body scattering wave functions. The first type evolves from an initial three-body incident wave describing three incident particles in continuum. The second type of the three-body scattering wave function evolves from a two-body incident wave corresponding to collision of a two-body bound state with a third particle.

The three-body incident wave represents the leading asymptotic terms of the total three-body scattering wave function [1, 2, 3]. The knowledge of the three-body incident wave is important for many reasons: as a leading term of the three-body wave function it can be used in calculations of the breakup matrix elements if the kinematics is such that the asymptotic region gives the leading contribution; the knowledge of the three-body incident wave is necessary in direct solution of the three-body Schrödinger equation for the scattering wave function of the first type. The asymptotic behavior of the three-body incident wave depends on the asymptotic region under consideration. In the asymptotic region where two particles, for example β and γ , are close to each other and far away from the third particle α , the three-body incident wave can be written as an asymptotic series in powers $1/\rho_\alpha$, where ρ_α is the distance between the c.m. of the system (β, γ) and the third particle α . The leading asymptotic terms $O(1)$ and $O(1/\rho_\alpha)$ of the three-body incident wave for charged particles have been obtained analytically in [2, 3]. These asymptotic terms satisfy the Schrödinger equation up to $O(1/\rho_\alpha^2)$. In this work we will derive all the leading asymptotic terms of the three charged particles incident wave of order $O(1/\rho_\alpha^2)$. Combined with the previously derived terms of order $O(1)$ and $O(1/\rho_\alpha)$ [2, 3], they provide the asymptotic solution of the Schrödinger equation for three charged particles in continuum up to terms $O(1/\rho_\alpha^3)$. The terms $O(1/\rho_\alpha^3)$ satisfy first order differential equations. It is worth mentioning that the terms $O(1/\rho_\alpha^3)$ are the next order terms compared to the three-body scattered wave which is $O(1/R^{5/2})$, where R is the hyperradius. This term, as well as the leading-order asymptotic terms of the three-body wave function of the second type have been given in Refs. [4, 5]. Practical ways of extracting the scattering and breakup amplitudes using these asymptotic wave functions have been presented in Refs. [6, 7].

The paper is organized in the following way. In Section I we introduce the three-body nomenclature and give the statement of the problem. In Section II we recall some of the important relations relevant to two-body scattering. In Sections III-V we present asymptotic solutions of the three-body Schrödinger equation in all orders which can be obtained analytically with the asymptotic method. Finally, Section F concludes the paper.

II. STATEMENT OF THE PROBLEM

We consider a non-relativistic three-body problem for charged particles of mass m_α and charge z_α , $\alpha = 1, 2, 3$ in the continuum state. We follow the notations used in Ref. [2]. The Greek letters stand for constituent particles of the three-body system or for the pair of two other particles. For example, α labels the particle or the pair $\beta + \gamma$. Such a supplemental notation is customary in few-body physics. The following conventional notations for the two body quantities are also used: $A_\alpha \equiv A_{\beta\gamma}$, where $\alpha \neq \beta \neq \gamma$. The Jacobi coordinates are determined as follows: \mathbf{r}_α

is the relative coordinate between particles β and γ , and \mathbf{k}_α is its canonically conjugated momentum. $\mu_\alpha = \frac{m_\beta m_\gamma}{m_{\beta\gamma}}$ is their reduced mass, $m_{\beta\gamma} = m_\beta + m_\gamma$. Similarly, $\boldsymbol{\rho}_\alpha$ is the relative coordinate between the c.m. of the pair (β, γ) and particle α , and \mathbf{q}_α is its canonically conjugated relative momentum. $M_\alpha = m_\alpha m_{\beta\gamma}/M$, $M = \sum_{\nu=1}^3 m_\nu$ is total mass of the three-body system. There are three sets of Jacobi coordinates $\mathbf{r}_\nu, \boldsymbol{\rho}_\nu$, where $\nu = \alpha, \beta, \gamma$. We frequently need the relations between the coordinates, and conjugate momenta for a channel $\nu = \beta, \gamma$ and the corresponding α -channel variables. They are given by the following relations

$$\begin{pmatrix} \boldsymbol{\rho}_\nu \\ \mathbf{r}_\nu \end{pmatrix} = \begin{pmatrix} -\frac{m_\alpha}{M-m_\nu} & \epsilon_{\nu\alpha} \frac{\mu_\nu}{M_\alpha} \\ -\epsilon_{\nu\alpha} & -\frac{m_\nu}{m_{\beta\gamma}} \end{pmatrix} \begin{pmatrix} \boldsymbol{\rho}_\alpha \\ \mathbf{r}_\alpha \end{pmatrix} \quad (1)$$

$$\begin{pmatrix} \mathbf{q}_\nu \\ \mathbf{k}_\nu \end{pmatrix} = \begin{pmatrix} -\frac{m_\nu}{m_{\beta\gamma}} & \epsilon_{\nu\alpha} \\ -\epsilon_{\nu\alpha} \frac{\mu_\alpha}{M_\nu} & -\frac{m_\alpha}{M-m_\nu} \end{pmatrix} \begin{pmatrix} \mathbf{q}_\alpha \\ \mathbf{k}_\alpha \end{pmatrix}, \quad (2)$$

where $\nu = \beta, \gamma$ and the antisymmetric symbol $\epsilon_{\alpha\nu} = -\epsilon_{\nu\alpha}$, with $\epsilon_{\alpha\nu} = 1$ for (α, ν) being a cyclic permutation of $(1, 2, 3)$, and $\epsilon_{\alpha\alpha} = 0$. The motion of the three particles is described by the Schrödinger equation in the configuration space

$$\{E - T_{\mathbf{r}_\alpha} - T_{\boldsymbol{\rho}_\alpha} - V\} \Psi_{\mathbf{k}_\alpha \mathbf{q}_\alpha}^{(+)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = 0, \quad (3)$$

where $V = \sum_{\nu=1}^3 V_\nu$, $V_\nu = V_\nu^C(\mathbf{r}_\nu) + V_\nu^N(\mathbf{r}_\nu)$. The Coulomb potential is given by $V_\alpha^C(\mathbf{r}_\alpha) = \frac{Z_\beta Z_\gamma e^2}{r_\alpha}$, $Z_\nu e$ is the charge of particle ν . Similarly, V_ν^N is the nuclear potential between the particles of the ν -pair, where $\nu = \alpha, \beta, \gamma$. $T_{\mathbf{r}_\alpha} = -\frac{\Delta_{\mathbf{r}_\alpha}}{2\mu_\alpha}$, is the kinetic energy operator for the relative motion of particles β and γ , and $T_{\boldsymbol{\rho}_\alpha} = -\frac{\Delta_{\boldsymbol{\rho}_\alpha}}{2M_\alpha}$ is the kinetic energy operator for the relative motion of particle α and the center of mass of the pair (β, γ) , respectively.

Our aim is to derive the asymptotic behavior of three-body incident wave up to terms $O(1/\rho_\alpha^3)$ in the asymptotic region Ω_α , where $r_\alpha/\rho_\alpha \rightarrow 0$ and $\rho_\alpha \rightarrow \infty$. This incident wave provides the leading asymptotic terms of the three-body scattering wave function of the first type. General asymptotic behavior of the three-body scattering wave function is given by [1]

$$\begin{aligned} \Psi_{\mathbf{k}_\alpha, \mathbf{q}_\alpha}^{(+)} &\approx \tilde{\Psi}_{\mathbf{k}_\alpha, \mathbf{q}_\alpha}^{(+)} + \sum_{\nu=\alpha, \beta, \gamma} \varphi_\nu(\mathbf{r}_\nu) \frac{\mathcal{M}_{3 \rightarrow 2}^{(\nu)}}{\rho_\nu} e^{i q_\nu \rho_\nu - i \bar{\eta}_\nu \ln(2q_\nu \rho_\nu)} \\ &\quad + \frac{\mathcal{M}_{3 \rightarrow 3}}{R^{5/2}} e^{i \kappa R - i \lambda_0 \ln(2\kappa R)}. \end{aligned} \quad (4)$$

Here the first term is the incident three-body wave, the sum over ν provides the two-body outgoing scattered waves and corresponds to the $3 \rightarrow 2$ processes. The last term describes the outgoing three-body scattered wave. Also, $\bar{\eta}_\alpha = (Z_\beta + Z_\gamma) Z_\alpha e^2 M_\alpha / q_\alpha$ is the Coulomb parameter for the Coulomb interaction between particles α and the center of mass of the system $\beta + \gamma$; the Coulomb parameter λ_0 is determined in Ref. [5]. We use the system of units such that $\hbar = c = 1$. Formally we can determine the incident wave as an asymptotic difference

$$\begin{aligned} \tilde{\Psi}_{\mathbf{k}_\alpha, \mathbf{q}_\alpha}^{(+)} &\approx \Psi_{\mathbf{k}_\alpha, \mathbf{q}_\alpha}^{(+)} - \sum_{\nu=\alpha, \beta, \gamma} \varphi_\nu(\mathbf{r}_\nu) \frac{\mathcal{M}_{3 \rightarrow 2}^{(\nu)}}{\rho_\nu} e^{i q_\nu \rho_\nu - i \bar{\eta}_\nu \ln(2q_\nu \rho_\nu)} \\ &\quad - \frac{\mathcal{M}_{3 \rightarrow 3}}{R^{5/2}} e^{i \kappa R - i \lambda_0 \ln(2\kappa R)}. \end{aligned} \quad (5)$$

From this equation it is clear that the three-body incident wave is a part of the full wave function, which does not contain the outgoing two- and three-body scattered waves. For better understanding of the three-body incident wave we consider first the two-body case.

III. ASYMPTOTIC TWO-BODY SCATTERING WAVE FUNCTION

We will be referring to the two-body Coulomb scattering throughout this work. Therefore we present here some important relations for the two-body scattering. Let us consider two charged particles with mass m_i and charge

$Z_i e$, $i = 1, 2$, interacting via the pure Coulomb potential $V = Z_1 Z_2 e^2 / r$. Scattering of two particles is described by the Schrödinger equation

$$\{E - H\} \psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = 0, \quad (6)$$

where $\eta = Z_1 Z_2 e^2 \mu / k$ is the Coulomb parameter, $E = k^2 / (2\mu)$ is the relative kinetic energy of the interacting particles 1 and 2, $H = -\Delta_{\mathbf{r}} / (2\mu) + V$ is two body Hamiltonian, and $\mu = m_1 m_2 / (m_1 + m_2)$ is reduced mass of particles 1 and 2. For the pure Coulomb interaction case Eq.(6) can be solved analytically. Substituting

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} N {}_1F_1(-i\eta, 1, i\zeta), \quad (7)$$

into Eq.(6) gives the differential equation for the confluent hypergeometric function (also called the Kummer function)

$$\left[\frac{\Delta_{\mathbf{r}}}{2\mu} + \frac{i\mathbf{k} \cdot \nabla_{\mathbf{r}}}{\mu} - V \right] {}_1F_1(-i\eta, 1, i\zeta) = 0, \quad (8)$$

$N = e^{-\pi\eta/2} \Gamma(1 + i\eta)$ is the normalization factor, and parabolic coordinate $\zeta = kr - \mathbf{k} \cdot \mathbf{r}$. ${}_1F_1(-i\eta, 1, i\zeta)$ is called the Kummer function because Eq. (8) rewritten in terms of $z = i\zeta$ becomes the Kummer differential equation [8, 9]:

$$z \frac{d^2 {}_1F_1(a, c; z)}{dz^2} + (c - z) \frac{d {}_1F_1(a, c; z)}{dz} - a {}_1F_1(a, c; z) = 0. \quad (9)$$

Here $a = -i\eta$, $c = 1$. Note that the Kummer function ${}_1F_1(a, c; z)$ is a regular solution at $\zeta = 0$ (or $r = 0$) of the Kummer equation. Correspondingly, $\psi_{\mathbf{k}}^{(+)}(\mathbf{r})$ given by Eq. (7) is the normalized regular solution of the two-body Coulomb scattering problem. The Kummer function can be expressed in terms of the Whittaker functions $W_{\lambda, \mu}(z)$ using Eqs. (9.220.3) and (9.233.2) [10]:

$$\begin{aligned} {}_1F_1(-i\eta, 1; i\zeta) &= \frac{1}{\Gamma(1 + i\eta)} e^{\pi\eta} \frac{1}{(i\zeta)^{1/2}} e^{i\zeta/2} W_{1/2 + i\eta}(i\zeta) \\ &+ \frac{1}{\Gamma(-i\eta)} e^{-i\pi(1/2 + i\eta)} \frac{1}{(i\zeta)^{1/2}} e^{i\zeta/2} W_{-1/2 - i\eta, 0}(e^{-i\pi} i\zeta). \end{aligned} \quad (10)$$

Each term of Eq. (10) also satisfies the Kummer differential equation (9) providing a singular solution. Substituting Eq. (10) into the Kummer equation leads to the Whittaker differential equation for each term:

$$\frac{d^2 W_{\lambda, 0}(z)}{dz^2} + \left(-\frac{1}{4} + \frac{\lambda}{z} + \frac{\frac{1}{4} - \nu^2}{z^2} \right) W_{\lambda, 0}(z) = 0. \quad (11)$$

Here $\lambda = \pm(1/2 + i\eta)$ and $z = \pm i\zeta$. Evidently that both Whittaker functions in Eq. (10) satisfy the same Whittaker equation because it is invariant under simultaneous transformation $z \rightarrow -z$, $\lambda \rightarrow -\lambda$. Coming back to the normalized regular solution of the Schrödinger equation we can present it as a sum of two singular solutions:

$$\begin{aligned} \psi_{\mathbf{k}}^{(+)}(\mathbf{r}) &= e^{i\mathbf{k} \cdot \mathbf{r}} N {}_1F_1(-i\eta, 1, i\zeta) \\ &= \psi_{\mathbf{k}}^{(0)}(\mathbf{r}) + \psi_{\mathbf{k}}^{(sc)}(\mathbf{r}). \end{aligned} \quad (12)$$

The first singular solution, as we will see below, is the incident wave

$$\psi_{\mathbf{k}}^{(0)}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} \mathcal{F}^{(1)}(\zeta), \quad (13)$$

and the second singular solution is the scattered wave

$$\psi_{\mathbf{k}}^{(sc)}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} \mathcal{F}^{(2)}(\zeta), \quad (14)$$

$$\mathcal{F}^{(1)}(\zeta) = e^{\frac{\pi\eta}{2}} (i\zeta)^{-\frac{1}{2}} e^{i\frac{\zeta}{2}} W_{i\eta + \frac{1}{2}, 0}(i\zeta), \quad (15)$$

$$\mathcal{F}^{(2)}(\zeta) = -i \frac{\Gamma(1 + i\eta)}{\Gamma(-i\eta)} e^{\frac{\pi\eta}{2}} (i\zeta)^{-\frac{1}{2}} e^{i\frac{\zeta}{2}} W_{-i\eta - \frac{1}{2}, 0}(e^{-i\pi} i\zeta). \quad (16)$$

Evidently that for $\eta = 0$ the incident wave becomes the plane wave $e^{i\mathbf{k}\cdot\mathbf{r}}$ and the scattered wave just disappears. It follows from Eq. (9.227) [10] that ($|z| > 0$)

$$W_{1/2,0}(z) = e^{-z/2} z^{1/2} \int_0^\infty dt e^{-t} \frac{1}{t+z}. \quad (17)$$

and from Eq. (6.922.2) [10]

$$W_{-1/2,0}(z) = e^{-z/2} z^{1/2} \int_0^\infty dt e^{-t} \frac{1}{t+z}. \quad (18)$$

Taking into account the asymptotic behaviour at $|z| \rightarrow \infty$ of the Whittaker function, Eq. (9.227) [10],

$$W_{\lambda,0}(z) \stackrel{|z| \rightarrow \infty}{\sim} z^\lambda e^{-z/2} \left[1 - \frac{(\lambda - 1/2)^2}{z} + O\left(\frac{1}{z^2}\right) \right], \quad (19)$$

we derive the asymptotic behavior of $\mathcal{F}^{(1)}(\zeta)$:

$$\mathcal{F}^{(1)}(i\zeta) \stackrel{|\zeta| \rightarrow \infty}{\sim} e^{i\eta \ln \zeta} \left[1 + O\left(\frac{1}{i\zeta}\right) \right]. \quad (20)$$

Correspondingly the asymptotic behavior of the Coulomb distorted incident wave

$$\psi_{\mathbf{k}}^{(0)}(\mathbf{r}) \stackrel{r \rightarrow \infty}{\sim} e^{i\mathbf{k}\cdot\mathbf{r}} e^{i\eta \ln \zeta} \left[1 + O\left(\frac{1}{i\zeta}\right) \right]. \quad (21)$$

The asymptotic behavior of $\mathcal{F}^{(2)}(\zeta)$ is given by

$$\mathcal{F}^{(2)}(i\zeta) \stackrel{\zeta \rightarrow \infty}{\sim} f^C \frac{e^{i\zeta}}{r} e^{-i\eta \ln 2kr} \left[1 + O\left(\frac{1}{i\zeta}\right) \right], \quad (22)$$

where f^C is the on-the-energy-shell Coulomb scattering amplitude:

$$f^C = -\eta \frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)} (-i)^{-i\eta} e^{\pi\eta/2} \frac{e^{-i\eta \ln \sin^2 \frac{\theta}{2}}}{2k \sin^2 \frac{\theta}{2}}. \quad (23)$$

The asymptotic behavior of the scattered wave is given by

$$\psi_{\mathbf{k}}^{(sc)}(\mathbf{r}) \stackrel{r \rightarrow \infty}{\sim} f^C \frac{e^{ikr}}{r} e^{-i\eta \ln 2kr} \left[1 + O\left(\frac{1}{i\zeta}\right) \right]. \quad (24)$$

Taking into account Eqs. (12), (21), (24) we get the asymptotic behavior of the Coulomb scattering wave function for a system of two particles in the coordinate space:

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) \stackrel{r \rightarrow \infty}{\sim} e^{i\mathbf{k}\cdot\mathbf{r}} e^{i\eta \ln \zeta} \left[1 + O\left(\frac{1}{i\zeta}\right) \right] + f^C \frac{e^{ikr}}{r} e^{-i\eta \ln 2kr} \left[1 + O\left(\frac{1}{i\zeta}\right) \right]. \quad (25)$$

Note that this asymptotic behavior is valid only for $|\zeta| \rightarrow \infty$. For $r \rightarrow \infty$ it is valid for all directions in the configuration space except for the so-called singular direction, for which $\hat{\mathbf{k}} \cdot \hat{\mathbf{r}} = 1$. Here $\hat{\mathbf{a}} = \mathbf{a}/a$.

One can observe a very interesting feature in the case of the two-body Coulomb scattering. The regular solution, according to Eq. (12), consists of two singular solutions, incident and scattered wave, each of them also satisfies the Schrödinger equation. Correspondingly, the asymptotic Coulomb scattering wave function consists of two terms. The first one, $e^{i\mathbf{k}\cdot\mathbf{r}} e^{i\eta \ln \zeta} (1 + O(\frac{1}{i\zeta}))$ is the asymptotic form of $e^{i\mathbf{k}\cdot\mathbf{r}} \mathcal{F}^{(1)}(i\zeta)$ and represents the Coulomb distorted incident wave. The Coulomb distortion not only generates a logarithmic phase factor $\eta \ln \zeta$ as an additional phase factor to the plane wave phase factor $\mathbf{k} \cdot \mathbf{r}$, but it also generates an infinite series in powers of $1/\zeta$. This is in contrast to the two-body scattering problem for particles interacting via short-range potentials, where the incident wave is given just by the plane wave. The second term in Eq. (25) is the asymptotic form for $e^{i\mathbf{k}\cdot\mathbf{r}} \mathcal{F}^{(2)}(i\zeta)$. It generates the outgoing two-body spherical wave times the Coulomb scattering amplitude and also contains a factor which can be written as an asymptotic expansion in powers of $1/\zeta$.

IV. ASYMPTOTIC THREE-BODY INCIDENT WAVE

After consideration of the incident wave for the two-body case, it is easier to proceed to the incident wave for the three-body case. By definition, the incident three-body wave is the part of the total three-body scattering wave function of the first type, which does not contain two- and three-body scattered waves. We have shown that the two-body incident wave is a singular solution of the two-body Schrödinger equation. It is naturally to ask whether the three-body incident wave is a solution of the three-body Schrödinger equation. An educated guess tells us that the answer may be "yes". First, the scattering wave function of the first type which consists of the three-body incident and scattered waves (two- and three-body) is a regular solution of the three-body Schrödinger equation. However there are also singular solutions of the three-body Schrödinger equation. And it is very plausible that the three-body incident wave is one of the singular solutions while the scattered wave represents another singular solution. However, we cannot prove it until an analytical expression for the three-body incident wave will be available.

Our goal in this work is to derive the asymptotic incident three-body wave function in the leading orders $O(1)$, $O(1/\rho_\alpha^2)$, $O(1/\rho_\alpha^3)$ in the asymptotic region Ω_α , where particles β and γ are close to each other and far away from particle α . We will demonstrate that the terms of order $O(1/\rho_\alpha^2)$ can be derived without explicit solution of the three-body Schrödinger equation. In principle the method we use can be applied to get even the higher order terms of the three-body incident wave but it is worth mentioning that the next order term in the asymptotic expansion of the three-body incident wave $O(1/\rho_\alpha^3)$ is inferior to the outgoing three-body scattered wave $O(1/R^{5/2})$. Hence for practical applications one need to know the three-body scattered wave before getting the term $O(1/\rho_\alpha^3)$ in the asymptotic expansion of the three-body incident wave. A knowledge of the three-body incident wave up to terms $O(1/\rho_\alpha^3)$ allows us to write down the leading asymptotic terms of the three-body scattering wave function of the first type in the asymptotic region Ω_α up to terms $O(1/\rho_\alpha^3)$. Note that the expressions for the asymptotic incident three-body wave in two other asymptotic regions Ω_β and Ω_γ can be derived by simple cyclic permutation of indexes α , β and γ . As we have mentioned earlier, the asymptotic incident three-body wave is the part of the total three-body scattering wave function of the first type, which does not contain two- and three-body scattered waves. This wave function should smoothly transform into the asymptotic incident three-body wave function in the asymptotic region Ω_0 . This smooth matching is an important part of the boundary conditions that provides a unique solution.

The leading asymptotic term of the three-body incident wave in Ω_0 derived by Redmond [11, 12] is given by

$$\Psi_{\mathbf{k}_\alpha, \mathbf{q}_\alpha}^{(0)(+)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = e^{i\mathbf{k}_\alpha \cdot \mathbf{r}_\alpha} e^{i\mathbf{q}_\alpha \cdot \boldsymbol{\rho}_\alpha} \prod_{\nu=\alpha, \beta, \gamma} e^{i\eta_\nu \ln \zeta_\nu}, \quad (26)$$

where

$$\zeta_\nu = k_\nu r_\nu - \mathbf{k}_\nu \cdot \mathbf{r}_\nu. \quad (27)$$

$$\eta_\alpha = \frac{Z_\beta Z_\gamma e^2 \mu_\alpha}{k_\alpha} \quad (28)$$

is the Coulomb parameter of particles β and γ , μ_α is the reduced mass of particles β and γ . It is the three-body Coulomb distorted plane wave. For practical applications Merkuriev [1], Garibotti and Miraglia [13] extended the asymptotic Redmond's term by substituting the confluent hypergeometric functions for the exponential Coulomb distortion factors. This extended wave function, often called the 3C wave function, is given by

$$\Psi_{\mathbf{k}_\alpha, \mathbf{q}_\alpha}^{(3C)(+)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = e^{i\mathbf{k}_\alpha \cdot \mathbf{r}_\alpha} e^{i\mathbf{q}_\alpha \cdot \boldsymbol{\rho}_\alpha} \prod_{\nu=\alpha, \beta, \gamma} F_\nu(\zeta_\nu), \quad (29)$$

where

$$F_\nu(\zeta_\nu) = N_\nu {}_1F_1(-i\eta_\nu, 1; i\zeta_\nu), \quad (30)$$

${}_1F_1(-i\eta_\nu, 1; i\zeta_\nu)$ is the confluent hypergeometric function and

$$N_\nu = e^{-\pi\eta_\nu/2} \Gamma(1 + i\eta_\nu). \quad (31)$$

Note that

$$\psi_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha) = e^{i\mathbf{k}_\alpha \cdot \mathbf{r}_\alpha} F_\nu(\zeta_\nu) \quad (32)$$

is the Coulomb scattering wave function of particles β and γ moving with the relative momentum \mathbf{k}_α and is well-behaved even in the singular directions ($\zeta_\nu < C$ for $r_\nu \rightarrow \infty$) where the Redmond's asymptotic term is not determined. If any of the particles is neutral, then the resulting asymptotic solution becomes the plane wave for the neutral particle and the exact two-body scattering wave function for the charged pair. However, neither Redmond's asymptotic term $\Psi_{\mathbf{k}_\alpha, \mathbf{q}_\alpha}^{(0)(+)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ nor the 3C wave function $\Psi_{\mathbf{k}_\alpha, \mathbf{q}_\alpha}^{(3C)(+)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ are asymptotic solutions of the Schrödinger equation in the asymptotic domains Ω_ν , $\nu = \alpha, \beta, \gamma$. Redmond's asymptotic term, by construction, satisfies the asymptotic Schrödinger equation up to terms $O(1/r_\alpha^2, 1/r_\beta^2, 1/r_\gamma^2)$. However, in the asymptotic region, Ω_ν , the distance between the particles of pair ν is limited: $r_\nu < C'$. Hence the terms $O(1/r_\nu)$ are not small and the potential V_ν^C in the Schrödinger equation has to be compensated exactly rather than asymptotically as happens when we use the Redmond's asymptotic wave function in Ω_0 . In the 3C wave function two very important effects are absent. Consider, for example, the asymptotic region Ω_α . In this region $r_\alpha \ll \rho_\alpha$. Hence the two-body relative motion of particles β and γ is distorted by the Coulomb field of the third particle α [2]. The second evident defect in the 3C function is the absence of the nuclear interaction between particles β and γ which can be close enough to each other in Ω_α . Nevertheless, the 3C wave function can be used as a starting point to derive the leading asymptotic terms of the three-body incident wave in Ω_α [2, 3], because this asymptotic three-body incident wave should match the Redmond's asymptotic term in Ω_0 . We will demonstrate now how important the condition of the matching of the asymptotic wave functions is on the border of different asymptotic regions [2].

In the Redmond's asymptotic incident wave three logarithmic phase factors appear, one phase factor for each pair rather than two phase factors in the factorized solution. It is a very important conclusion. In all the conventional approaches for breakup processes, including coupled channels codes like FRESKO, the three-body scattering wave function is approximated by the factorized one. From the consideration above, it is clear that if Coulomb interactions are important, such an approximation is not accurate. If the interactions are short-range, the factorized solution matches the asymptotic solution in Ω_0 and is justified in the asymptotic region Ω_α . It has been shown in [2, 3] that the actual asymptotic solution of the asymptotic Schrödinger equation $\Psi_{\mathbf{k}_\alpha, \mathbf{q}_\alpha}^{(as)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$, which matches the Redmond's asymptotic term in Ω_0 , cannot be written in a factorized form and has a quite complicated behavior. In [2, 3] all the leading asymptotic terms up to $O(1/\rho_\alpha^2)$ of the asymptotic wave function $\Psi_{\mathbf{k}_\alpha, \mathbf{q}_\alpha}^{(as)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ have been derived in the asymptotic region Ω_α . In this work we will present a derivation of the expansion of the asymptotic wave function, $\Psi_{\mathbf{k}_\alpha, \mathbf{q}_\alpha}^{(as)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$, up to terms $O(1/\rho_\alpha^3)$. The derived asymptotic expansion contains all the terms $O(1)$, $O(1/\rho_\alpha)$ and $O(1/\rho_\alpha^2)$. Since we are looking for the terms $O(1/\rho_\alpha^2)$, we need to keep the terms up to $O(1/\rho_\alpha^3)$. Instead of the asymptotic expansion of the Coulomb potentials $V_\beta^C(\mathbf{r}_\beta)$ and $V_\gamma^C(\mathbf{r}_\gamma)$ in terms of $1/\rho_\alpha$, we will start our derivation from the exact three-body Schrödinger equation (3). The terms of $O(1/\rho_\alpha^3)$ will be dropped later. The asymptotic wave function in Ω_α should match the asymptotic wave function in Ω_0 . The 3C wave function satisfies Eq.(3) up to terms $O(1/r_\alpha^2, 1/\rho_\alpha^2)$ and we can use it as the initial wave function. However, this wave function should be modified to satisfy the Schrödinger equation in Ω_α . Note that usually in the literature it is assumed that the Redmond's asymptotic term satisfies the Schrödinger equation in Ω_0 in the leading order only. First we will show that the 3C wave function satisfies the Schrödinger equation in Ω_0 up to terms of order $O(1/r_\nu^2)$. To this end we just substitute the

3C wave function (29) into the Schrödinger equation (3):

$$\begin{aligned}
& (E - T_{\mathbf{r}_\alpha} - T_{\boldsymbol{\rho}_\alpha} - V)[e^{i\mathbf{k}_\alpha \cdot \mathbf{r}_\alpha + i\mathbf{q}_\alpha \cdot \boldsymbol{\rho}_\alpha} \varphi_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha) \varphi_{\mathbf{k}_\beta}(\mathbf{r}_\beta) \varphi_{\mathbf{k}_\gamma}(\mathbf{r}_\gamma)] \\
& = e^{i\mathbf{k}_\alpha \cdot \mathbf{r}_\alpha + i\mathbf{q}_\alpha \cdot \boldsymbol{\rho}_\alpha} \varphi_{\mathbf{k}_\beta}(\mathbf{r}_\beta) \varphi_{\mathbf{k}_\gamma}(\mathbf{r}_\gamma) \left[\frac{\Delta_{\mathbf{r}_\alpha}}{2\mu_\alpha} + \frac{i\mathbf{k}_\alpha \cdot \nabla_{\mathbf{r}_\alpha}}{\mu_\alpha} - V_\alpha \right. \\
& \quad + \frac{\Delta_{\boldsymbol{\rho}_\alpha}}{2M_\alpha} + \frac{i[\mathbf{q}_\alpha - i \sum_{\nu=\beta,\gamma} \nabla_{\boldsymbol{\rho}_\alpha} \ln \varphi_{\mathbf{k}_\nu}] \cdot \nabla_{\boldsymbol{\rho}_\alpha}}{M_\alpha} \\
& \quad + \frac{\nabla_{\mathbf{r}_\alpha} \varphi_{\mathbf{k}_\gamma} \cdot \nabla_{\mathbf{r}_\alpha} \varphi_{\mathbf{k}_\beta}}{\mu_\alpha \varphi_{\mathbf{k}_\beta} \varphi_{\mathbf{k}_\gamma}} + \frac{\nabla_{\boldsymbol{\rho}_\alpha} \varphi_{\mathbf{k}_\gamma} \cdot \nabla_{\boldsymbol{\rho}_\alpha} \varphi_{\mathbf{k}_\beta}}{M_\alpha \varphi_{\mathbf{k}_\beta} \varphi_{\mathbf{k}_\gamma}} \left. \right] \varphi_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha) \\
& + e^{i\mathbf{k}_\beta \cdot \mathbf{r}_\beta + i\mathbf{q}_\beta \cdot \boldsymbol{\rho}_\beta} \varphi_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha) \varphi_{\mathbf{k}_\gamma}(\mathbf{r}_\gamma) \left[\frac{\Delta_{\mathbf{r}_\beta}}{2\mu_\beta} + \frac{i\mathbf{k}_\beta \cdot \nabla_{\mathbf{r}_\beta}}{\mu_\beta} - V_\beta \right. \\
& \quad + \frac{\Delta_{\boldsymbol{\rho}_\beta}}{2M_\beta} + \frac{i[\mathbf{q}_\beta - i \sum_{\tau=\alpha,\gamma} \nabla_{\boldsymbol{\rho}_\beta} \ln \varphi_{\mathbf{k}_\tau}] \cdot \nabla_{\boldsymbol{\rho}_\beta}}{M_\beta} \\
& \quad + \frac{\nabla_{\mathbf{r}_\beta} \varphi_{\mathbf{k}_\gamma} \cdot \nabla_{\mathbf{r}_\beta} \varphi_{\mathbf{k}_\alpha}}{\mu_\beta \varphi_{\mathbf{k}_\alpha} \varphi_{\mathbf{k}_\gamma}} + \frac{\nabla_{\boldsymbol{\rho}_\beta} \varphi_{\mathbf{k}_\gamma} \cdot \nabla_{\boldsymbol{\rho}_\beta} \varphi_{\mathbf{k}_\alpha}}{M_\beta \varphi_{\mathbf{k}_\alpha} \varphi_{\mathbf{k}_\gamma}} \left. \right] \varphi_{\mathbf{k}_\beta}(\mathbf{r}_\beta) \\
& + e^{i\mathbf{k}_\gamma \cdot \mathbf{r}_\gamma + i\mathbf{q}_\gamma \cdot \boldsymbol{\rho}_\gamma} \varphi_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha) \varphi_{\mathbf{k}_\beta}(\mathbf{r}_\beta) \left[\frac{\Delta_{\mathbf{r}_\gamma}}{2\mu_\gamma} + \frac{i\mathbf{k}_\gamma \cdot \nabla_{\mathbf{r}_\gamma}}{\mu_\gamma} - V_\gamma \right. \\
& \quad + \frac{\Delta_{\boldsymbol{\rho}_\gamma}}{2M_\gamma} + \frac{i[\mathbf{q}_\gamma - i \sum_{\omega=\alpha,\beta} \nabla_{\boldsymbol{\rho}_\gamma} \ln \varphi_{\mathbf{k}_\omega}] \cdot \nabla_{\boldsymbol{\rho}_\gamma}}{M_\gamma} \\
& \quad + \frac{\nabla_{\mathbf{r}_\gamma} \varphi_{\mathbf{k}_\beta} \cdot \nabla_{\mathbf{r}_\gamma} \varphi_{\mathbf{k}_\alpha}}{\mu_\gamma \varphi_{\mathbf{k}_\alpha} \varphi_{\mathbf{k}_\beta}} + \frac{\nabla_{\boldsymbol{\rho}_\gamma} \varphi_{\mathbf{k}_\beta} \cdot \nabla_{\boldsymbol{\rho}_\gamma} \varphi_{\mathbf{k}_\alpha}}{M_\gamma \varphi_{\mathbf{k}_\alpha} \varphi_{\mathbf{k}_\beta}} \left. \right] \varphi_{\mathbf{k}_\gamma}(\mathbf{r}_\gamma). \tag{33}
\end{aligned}$$

Here

$$\varphi_{\mathbf{k}_\nu}(\mathbf{r}_\nu) = N_\nu F(-i\eta_\nu, 1; i\zeta_\nu) = \mathcal{F}_\nu^{(1)}(i\zeta_\nu) + \mathcal{F}_\nu^{(2)}(i\zeta_\nu). \tag{34}$$

Taking into account

$$\left[\frac{\Delta_{\mathbf{r}_\nu}}{2\mu_\nu} + \frac{i\mathbf{k}_\nu \cdot \nabla_{\mathbf{r}_\nu}}{\mu_\nu} - V_\nu \right] \varphi_{\mathbf{k}_\nu}(\mathbf{r}_\nu) = 0 \tag{35}$$

we derive

$$\begin{aligned}
& (E - T_{\mathbf{r}_\alpha} - T_{\boldsymbol{\rho}_\alpha} - V)[e^{i\mathbf{k}_\alpha \cdot \mathbf{r}_\alpha + i\mathbf{q}_\alpha \cdot \boldsymbol{\rho}_\alpha} \varphi_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha) \varphi_{\mathbf{k}_\beta}(\mathbf{r}_\beta) \varphi_{\mathbf{k}_\gamma}(\mathbf{r}_\gamma)] \\
& = O(1/r_\alpha^2, 1/r_\beta^2, 1/r_\gamma^2). \tag{36}
\end{aligned}$$

We did not use any approximation to get Eq. 36. Thus the 3C wave function indeed satisfies the Schrödinger equation in Ω_0 up to the terms $O(1/r_\alpha^2, 1/r_\beta^2, 1/r_\gamma^2)$, i. e. after substitution of the 3C wave function into the Schrödinger equation all the terms of order $O(1)$ and $O(1/r_\alpha)$ are exactly compensated. Hence the 3C wave function can be used as a starting wave function with a proper modifications to look for an asymptotic solution in Ω_α . Taking into account Eq. (34) we can rewrite the 3C wave function as in a form which is suitable for consideration in the Ω_α asymptotic domain:

$$\begin{aligned}
& \Psi_{\mathbf{k}_\alpha, \mathbf{q}_\alpha}^{(3C)(+)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = e^{i\mathbf{k}_\alpha \cdot \mathbf{r}_\alpha} e^{i\mathbf{q}_\alpha \cdot \boldsymbol{\rho}_\alpha} \\
& \times [\mathcal{F}_\beta^{(1)}(i\zeta_\beta) \mathcal{F}_\gamma^{(1)}(i\zeta_\gamma) N_\alpha F_\alpha(i\zeta_\alpha) + \mathcal{F}_\beta^{(2)}(i\zeta_\beta) \mathcal{F}_\gamma^{(1)}(i\zeta_\gamma) N_\alpha F_\alpha(i\zeta_\alpha) \\
& + \mathcal{F}_\beta^{(1)}(i\zeta_\beta) \mathcal{F}_\gamma^{(2)}(i\zeta_\gamma) N_\alpha F_\alpha(i\zeta_\alpha) + \mathcal{F}_\beta^{(2)}(i\zeta_\beta) \mathcal{F}_\gamma^{(2)}(i\zeta_\gamma) N_\alpha F_\alpha(i\zeta_\alpha)]. \tag{37}
\end{aligned}$$

Here, asymptotically, for $|\zeta_\nu| \rightarrow \infty$, the first term $\mathcal{F}_\nu^{(1)}(\zeta_\nu) \sim O(1)$ and the second term $\mathcal{F}_\nu^{(2)}(\zeta_\nu) \sim O(1/\zeta_\nu)$. Hence in the asymptotic domain Ω_α $\mathcal{F}_\nu^{(1)}(\zeta_\nu)$ and $\mathcal{F}_\nu^{(2)}(\zeta_\nu)$, $\nu = \beta, \gamma$, can be treated asymptotically while $\varphi_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha)$ should be considered explicitly, because Ω_α includes the region, where r_α is limited. Moreover, in the asymptotic region Ω_α the relative motion of particles β and γ is distorted by the third particle α due to the long-range Coulomb interaction. It means that the wave function of the relative motion of particles β and γ in Ω_α will be different from

the wave function $e^{i\mathbf{k}_\alpha \cdot \mathbf{r}_\alpha} N_\alpha F_\alpha(i\zeta_\alpha)$ describing the relative motion of particles β and γ in the absence of the third particle. Since interacting particles β and γ can be close to each other in Ω_α , their nuclear interaction should also be taken into account. Following [3] we replace each $N_\alpha F_\alpha(i\zeta_\alpha)$ in Eq. (38) by the corresponding unknown function $\varphi_\alpha^{(nm)}(\mathbf{r}_\alpha)$, $n, m = 1, 2$:

$$\begin{aligned} \Psi_{\mathbf{k}_\alpha, \mathbf{q}_\alpha}^{(as)(+)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) &= e^{i\mathbf{k}_\alpha \cdot \mathbf{r}_\alpha} e^{i\mathbf{q}_\alpha \cdot \boldsymbol{\rho}_\alpha} \\ &\times [\mathcal{F}_\beta^{(1)}(i\zeta_\beta) \mathcal{F}_\gamma^{(1)}(i\zeta_\gamma) \varphi_\alpha^{(11)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) + \mathcal{F}_\beta^{(2)}(i\zeta_\beta) \mathcal{F}_\gamma^{(1)}(i\zeta_\gamma) \varphi_\alpha^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) \\ &+ \mathcal{F}_\beta^{(1)}(i\zeta_\beta) \mathcal{F}_\gamma^{(2)}(i\zeta_\gamma) \varphi_\alpha^{(12)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) + \mathcal{F}_\beta^{(2)}(i\zeta_\beta) \mathcal{F}_\gamma^{(2)}(i\zeta_\gamma) \varphi_\alpha^{(22)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)]. \end{aligned} \quad (38)$$

Derivation of $\varphi_\alpha^{(nm)}(\mathbf{r}_\alpha)$, $n, m = 1, 2$ is our final goal. Now we substitute Eq. (38) into the Schrödinger equation (3). When substituting Eq. (38) into the Schrödinger equation we assume that each term of the sum (38) satisfies the Schrödinger equation. Moreover, as we will see, each function $\varphi_\alpha(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ depends on the preceding functions $\mathcal{F}_\beta^{(n)}(i\zeta_\beta) \mathcal{F}_\gamma^{(m)}(i\zeta_\gamma)$ where $n, m = 1, 2$, i.e. for each term in (38) the modification is different. We also take into account that

$$\left(\frac{1}{2\mu_\nu} \Delta_{\mathbf{r}_\nu} + i \frac{1}{\mu_\nu} \mathbf{k}_\nu \cdot \nabla_{\mathbf{r}_\nu} - V_\nu^C \right) \mathcal{F}_\nu^{(1,2)}(i\zeta_\nu) = 0. \quad (39)$$

Substitution of the first term of Eq. (38) into the Schrödinger equation generates the equation for $\varphi_\alpha^{(11)}(\mathbf{r}_\alpha)$:

$$\begin{aligned} &\mathcal{F}_\beta^{(1)}(i\zeta_\beta) \mathcal{F}_\gamma^{(1)}(i\zeta_\gamma) \left[\frac{1}{2\mu_\alpha} \Delta_{\mathbf{r}_\alpha} + \frac{1}{2M_\alpha} \Delta_{\boldsymbol{\rho}_\alpha} + i \frac{1}{\mu_\alpha} \mathbf{k}_\alpha \cdot \nabla_{\mathbf{r}_\alpha} + i \frac{1}{M_\alpha} \mathbf{q}_\alpha \cdot \nabla_{\boldsymbol{\rho}_\alpha} + \right. \\ &\frac{1}{\mu_\alpha} \sum_{\nu=\beta, \gamma} \nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\nu^{(1)}(i\zeta_\nu) \cdot \nabla_{\mathbf{r}_\alpha} + \frac{1}{M_\alpha} \sum_{\nu=\beta, \gamma} \nabla_{\boldsymbol{\rho}_\alpha} \ln \mathcal{F}_\nu^{(1)}(i\zeta_\nu) \cdot \nabla_{\boldsymbol{\rho}_\alpha} - V_\alpha(\mathbf{r}_\alpha) + \\ &\left. \frac{1}{\mu_\alpha} \nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\beta^{(1)}(i\zeta_\beta) \cdot \nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\gamma^{(1)}(i\zeta_\gamma) + \frac{1}{M_\alpha} \nabla_{\boldsymbol{\rho}_\alpha} \ln \mathcal{F}_\beta^{(1)}(i\zeta_\beta) \cdot \nabla_{\boldsymbol{\rho}_\alpha} \ln \mathcal{F}_\gamma^{(1)}(i\zeta_\gamma) \right] \\ &\times \varphi_\alpha^{(11)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = 0. \end{aligned} \quad (40)$$

Since particles β and γ are allowed to be close in Ω_α their interaction potential is given by the sum of the Coulomb and nuclear potentials. Now we will simplify this equation by dropping all the terms $O(1/\rho_\alpha^3)$ and explicitly compensate all the terms $O(1)$, $O(1/\rho_\alpha)$, $O(1/\rho_\alpha^2)$. We consider only the nonsingular directions, i. e. $\hat{\mathbf{k}}_\nu \cdot \hat{\mathbf{r}}_\nu \neq 1$, $\nu = \beta, \gamma$. To analyze the fifth term in the brackets we use equations

$$\mathcal{F}_\nu^{(1)}(i\zeta_\nu) = \tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_\nu) [1 - i \frac{\eta_\nu^2}{\zeta_\nu} + O(1/\zeta_\nu^2)], \quad (41)$$

$$\tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_\nu) = e^{i\eta_\nu \ln \zeta_\nu}, \quad (42)$$

$$\nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\nu^{(1)}(i\zeta_\nu) = \nabla_{\mathbf{r}_\alpha} \ln \tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_\nu) - i \frac{m_\nu}{m_{\beta\gamma}} \frac{\eta_\nu^2}{k_\nu r_\nu^2} \frac{\hat{\mathbf{r}}_\nu - \hat{\mathbf{k}}_\nu}{(1 - \hat{\mathbf{k}}_\nu \cdot \hat{\mathbf{r}}_\nu)^2} + O(1/r_\nu^3), \quad (43)$$

$$\begin{aligned} \nabla_{\mathbf{r}_\alpha} \ln \tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_\nu) &= \nabla_{\mathbf{r}_\alpha} e^{\frac{m_\nu}{m_{\beta\gamma}} \epsilon_{\nu\alpha} \mathbf{r}_\alpha \cdot \nabla_{\boldsymbol{\rho}_\alpha}} \ln \tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_{\nu\alpha}) \\ &= \epsilon_{\nu\alpha} \frac{m_\nu}{m_{\beta\gamma}} \nabla_{\boldsymbol{\rho}_\alpha} \ln \tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_{\nu\alpha}) + \frac{m_\nu^2}{m_{\beta\gamma}^2} (\mathbf{r}_\alpha \cdot \nabla_{\boldsymbol{\rho}_\alpha}) \nabla_{\boldsymbol{\rho}_\alpha} \ln \tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_{\nu\alpha}), \end{aligned} \quad (44)$$

$$\nabla_{\boldsymbol{\rho}_\alpha} \ln \tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_{\nu\alpha}) = i\eta_\nu \epsilon_{\nu\alpha} \frac{1}{\rho_\alpha} \frac{\hat{\mathbf{k}}_\nu - \epsilon_{\alpha\nu} \hat{\boldsymbol{\rho}}_\alpha}{1 - \epsilon_{\alpha\nu} \hat{\mathbf{k}}_\nu \cdot \hat{\boldsymbol{\rho}}_\alpha} + O\left(\frac{1}{\rho_\alpha^2}\right), \quad (45)$$

$$\nabla_{\mathbf{r}_\alpha} \left[-i \frac{\eta_\nu^2}{\zeta_\nu} \right] = i\eta_\nu^2 \frac{m_\nu}{m_{\beta\gamma}} \frac{1}{k_\nu \rho_\alpha^2} \frac{\hat{\mathbf{k}}_\nu - \epsilon_{\alpha\nu} \hat{\boldsymbol{\rho}}_\alpha}{(1 - \epsilon_{\alpha\nu} \hat{\mathbf{k}}_\nu \cdot \hat{\boldsymbol{\rho}}_\alpha)^2} + O\left(\frac{1}{\rho_\alpha^3}\right). \quad (46)$$

To estimate the sixth and the ninth terms we use equations

$$\nabla_{\rho_\alpha} \ln \mathcal{F}_\nu^{(1)}(i\zeta_\nu) = i\eta_\nu \frac{1}{r_\nu} \epsilon_{\nu\alpha} \frac{\hat{\mathbf{k}}_\nu - \hat{\mathbf{r}}_\nu}{1 - \hat{\mathbf{k}}_\nu \cdot \hat{\mathbf{r}}_\nu} + O\left(\frac{1}{r_\nu^2}\right) \quad (47)$$

$$= i\eta_\nu \epsilon_{\nu\alpha} \frac{1}{\rho_\alpha} \frac{\hat{\mathbf{k}}_\nu - \epsilon_{\alpha\nu} \hat{\rho}_\alpha}{1 - \epsilon_{\alpha\nu} \hat{\mathbf{k}}_\nu \cdot \hat{\rho}_\alpha} + O\left(\frac{1}{\rho_\alpha^2}\right). \quad (48)$$

To estimate the eighth term we use equation

$$\nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\nu^{(1)}(i\zeta_\nu) = i\eta_\nu \frac{m_\nu}{m_{\beta\gamma}} \frac{1}{r_\nu} \frac{\hat{\mathbf{k}}_\nu - \hat{\mathbf{r}}_\nu}{1 - \hat{\mathbf{k}}_\nu \cdot \hat{\mathbf{r}}_\nu}. \quad (49)$$

Note that in Ω_α radius r_α is limited *a priori* (more strictly, it is allowed to grow but slower than ρ_α). That is why we cannot use an asymptotic expansion in terms of $1/\zeta_\alpha$ in the asymptotic region Ω_α . Eqs (44), (45), (46) and (48) are valid only in Ω_α , while Eqs (43), (47) and (49) are valid both in Ω_0 and Ω_α .

Thus we reduced a three-body problem in the asymptotic domain Ω_α to a two-body problem: we need to find a solution of Eq. (40), which describes the relative motion of particles β and γ in the presence of the third particle α , which is far away, but it still distorts the relative motion of particles β and γ due to the long-range Coulomb interaction. This distortion results in the dependence of $\varphi_\alpha^{(11)}(\mathbf{r}_\alpha, \rho_\alpha)$ on ρ_α . When ρ_α increases this distortion should be weakened. Hence, $\varphi_\alpha^{(11)}(\mathbf{r}_\alpha, \rho_\alpha)$ actually depends on $1/\rho_\alpha$ and

$$\nabla_{\rho_\alpha} \varphi_\alpha^{(11)}(\mathbf{r}_\alpha, \rho_\alpha) \sim \frac{1}{\rho_\alpha^2}. \quad (50)$$

Because of that we may drop the second and sixth terms in Eq. (40) and rewrite it in the form

$$\begin{aligned} & \left[\frac{1}{2\mu_\alpha} \Delta_{\mathbf{r}_\alpha} + i \frac{1}{\mu_\alpha} \mathbf{k}_\alpha \cdot \nabla_{\mathbf{r}_\alpha} + i \frac{1}{M_\alpha} \mathbf{q}_\alpha \cdot \nabla_{\rho_\alpha} + \frac{1}{\mu_\alpha} \sum_{\nu=\beta,\gamma} \nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\nu^{(1)}(i\zeta_\nu) \cdot \nabla_{\mathbf{r}_\alpha} \right. \\ & \quad \left. - V_\alpha(\mathbf{r}_\alpha) + \frac{1}{\mu_\alpha} \nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\beta^{(1)}(i\zeta_\beta) \cdot \nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\gamma^{(1)}(i\zeta_\gamma) \right. \\ & \quad \left. + \frac{1}{M_\alpha} \nabla_{\rho_\alpha} \ln \mathcal{F}_\beta^{(1)}(i\zeta_\beta) \cdot \nabla_{\rho_\alpha} \ln \mathcal{F}_\gamma^{(1)}(i\zeta_\gamma) \right] \varphi_\alpha^{(11)}(\mathbf{r}_\alpha, \rho_\alpha) = 0. \end{aligned} \quad (51)$$

The last two terms are of $O(1/\rho_\alpha^2)$. Note that to satisfy this equation up to terms of $O(1/\rho_\alpha^3)$ all the terms of $O(1/\rho_\alpha^2)$ must be compensated. Taking into account Eqs (44) and (46) we can rewrite Eq. (51) as

$$\begin{aligned} & \left[\frac{1}{2\mu_\alpha} \Delta_{\mathbf{r}_\alpha} + i \frac{1}{\mu_\alpha} \mathbf{k}_\alpha^{(11)}(\rho_\alpha) \cdot \nabla_{\mathbf{r}_\alpha} + i \frac{1}{M_\alpha} \mathbf{q}_\alpha \cdot \nabla_{\rho_\alpha} \right. \\ & \quad \left. + \frac{1}{\mu_\alpha} \sum_{\nu=\beta,\gamma} \frac{m_\nu^2}{m_{\beta\gamma}^2} (\mathbf{r}_\alpha \cdot \nabla_{\rho_\alpha}) (\nabla_{\rho_\alpha} \ln \tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_{\nu\alpha}) \cdot \nabla_{\mathbf{r}_\alpha}) - V_\alpha(\mathbf{r}_\alpha) \right. \\ & \quad \left. + (\epsilon_{\beta\alpha} \epsilon_{\gamma\alpha} \frac{1}{m_{\beta\gamma}} + \frac{1}{M_\alpha}) \nabla_{\rho_\alpha} \ln \mathcal{F}_\beta^{(1)}(i\zeta_{\beta\alpha}) \cdot \nabla_{\rho_\alpha} \ln \mathcal{F}_\gamma^{(1)}(i\zeta_{\gamma\alpha}) \right] \\ & \quad \times \varphi_\alpha^{(11)}(\mathbf{r}_\alpha, \rho_\alpha) = O(1/\rho_\alpha^3). \end{aligned} \quad (52)$$

We introduced here a new local momentum

$$\mathbf{k}_\alpha^{(11)} = \mathbf{k}_\alpha - i \sum_{\nu=\beta,\gamma} \frac{m_\nu}{m_{\beta\gamma}} \left[\epsilon_{\nu\alpha} \nabla_{\rho_\alpha} \ln \tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_{\nu\alpha}) + i\eta_\nu^2 \frac{1}{k_\nu \rho_\alpha^2} \frac{\hat{\mathbf{k}}_\nu - \epsilon_{\alpha\nu} \hat{\rho}_\alpha}{(1 - \epsilon_{\alpha\nu} \hat{\mathbf{k}}_\nu \cdot \hat{\rho}_\alpha)^2} \right]. \quad (53)$$

Note that variables $\nabla_{\mathbf{r}_\alpha}$ and ∇_{ρ_α} are mixed up only in the fourth term of Eq. (52). We are looking for a solution in the form

$$\varphi_\alpha^{(11)}(\mathbf{r}_\alpha, \rho_\alpha) = \varphi_{\alpha(0)}^{(11)}(\mathbf{r}_\alpha, \rho_\alpha) \left(1 + \frac{\chi(\hat{\rho}_\alpha)}{\rho_\alpha} \right) + \frac{\varphi_{\alpha(1)}^{(11)}(\mathbf{r}_\alpha, \rho_\alpha)}{\rho_\alpha^2}, \quad (54)$$

where $\varphi_{\alpha(0)}^{(11)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ is a solution of

$$\left[\frac{1}{2\mu_\alpha} \boldsymbol{\Delta}_{\mathbf{r}_\alpha} + i \frac{1}{\mu_\alpha} \mathbf{k}_\alpha^{(11)}(\boldsymbol{\rho}_\alpha) \cdot \nabla_{\mathbf{r}_\alpha} - V_\alpha(\mathbf{r}_\alpha) \right] \varphi_{\alpha(0)}^{(11)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = 0. \quad (55)$$

$\chi(\hat{\boldsymbol{\rho}}_\alpha) \sim O(1)$ and is a solution of the first order differential equation

$$\begin{aligned} & i \frac{1}{M_\alpha} \mathbf{q}_\alpha \cdot \nabla_{\boldsymbol{\rho}_\alpha} \frac{\chi(\hat{\boldsymbol{\rho}}_\alpha)}{\rho_\alpha} \\ &= -(\epsilon_{\beta\alpha} \epsilon_{\gamma\alpha} \frac{1}{m_{\beta\gamma}} + \frac{1}{M_\alpha}) \nabla_{\boldsymbol{\rho}_\alpha} \ln \tilde{\mathcal{F}}_\beta^{(1)}(i\zeta_{\beta\alpha}) \cdot \nabla_{\boldsymbol{\rho}_\alpha} \ln \tilde{\mathcal{F}}_\gamma^{(1)}(i\zeta_{\gamma\alpha}). \end{aligned} \quad (56)$$

Finally $\varphi_{\alpha(1)}^{(11)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) \sim O(1)$ is a solution of the inhomogeneous equation

$$\begin{aligned} & \left[\frac{1}{2\mu_\alpha} \boldsymbol{\Delta}_{\mathbf{r}_\alpha} + i \frac{1}{\mu_\alpha} \mathbf{k}_\alpha^{(11)} \cdot \nabla_{\mathbf{r}_\alpha} - V_\alpha(\mathbf{r}_\alpha) \right] \varphi_{\alpha(1)}^{(11)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = -i \frac{\rho_\alpha^2}{M_\alpha} \mathbf{q}_\alpha \cdot \nabla_{\boldsymbol{\rho}_\alpha} \varphi_{\alpha(0)}^{(11)}(\mathbf{r}_\alpha) \\ & - \frac{\rho_\alpha^2}{\mu_\alpha} \sum_{\nu=\beta,\gamma} \frac{m_\nu^2}{m_{\beta\gamma}^2} (\mathbf{r}_\alpha \cdot \nabla_{\boldsymbol{\rho}_\alpha}) \nabla_{\boldsymbol{\rho}_\alpha} \ln \tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_{\nu\alpha}) \cdot \nabla_{\mathbf{r}_\alpha} \varphi_{\alpha(0)}^{(11)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha). \end{aligned} \quad (57)$$

Note that all the equations (55), (56) and (57) are "two-body" differential equations. On the left hand side they contain gradients and Laplacians over only one of the variables, \mathbf{r}_α or $\boldsymbol{\rho}_\alpha$. Therefore these equations can easily be solved numerically.

Now we consider the second term of Eq. (38). It satisfies the equation

$$\begin{aligned} & \mathcal{F}_\beta^{(2)}(i\zeta_\beta) \mathcal{F}_\gamma^{(1)}(i\zeta_\gamma) \left[\frac{1}{2\mu_\alpha} \boldsymbol{\Delta}_{\mathbf{r}_\alpha} + \frac{1}{2M_\alpha} \boldsymbol{\Delta}_{\boldsymbol{\rho}_\alpha} + i \frac{1}{\mu_\alpha} \mathbf{k}_\alpha \cdot \nabla_{\mathbf{r}_\alpha} + i \frac{1}{M_\alpha} \mathbf{q}_\alpha \cdot \nabla_{\boldsymbol{\rho}_\alpha} + \right. \\ & \frac{1}{\mu_\alpha} [\nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\beta^{(2)}(i\zeta_\beta) + \nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\gamma^{(1)}(i\zeta_\gamma)] \cdot \nabla_{\mathbf{r}_\alpha} \\ & + \frac{1}{M_\alpha} [\nabla_{\boldsymbol{\rho}_\alpha} \ln \mathcal{F}_\beta^{(2)}(i\zeta_\beta) + \nabla_{\boldsymbol{\rho}_\alpha} \ln \mathcal{F}_\gamma^{(1)}(i\zeta_\gamma)] \cdot \nabla_{\boldsymbol{\rho}_\alpha} - V_\alpha(\mathbf{r}_\alpha) + \\ & \frac{1}{\mu_\alpha} \nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\beta^{(2)}(i\zeta_\beta) \cdot \nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\gamma^{(1)}(i\zeta_\gamma) + \frac{1}{M_\alpha} \nabla_{\boldsymbol{\rho}_\alpha} \ln \mathcal{F}_\beta^{(2)}(i\zeta_\beta) \cdot \nabla_{\boldsymbol{\rho}_\alpha} \ln \mathcal{F}_\gamma^{(1)}(i\zeta_\gamma) \\ & \left. \times \varphi_{\alpha(1)}^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = O(1/\rho_\alpha^3). \right] \end{aligned} \quad (58)$$

Here, in the nonsingular directions ($\hat{\mathbf{k}}_\nu \cdot \hat{\mathbf{r}}_\nu \neq 1, \nu \neq \alpha$)

$$\mathcal{F}_\nu^{(2)}(i\zeta_\nu) \stackrel{\zeta_\nu \rightarrow \infty}{\sim} \eta_\nu \frac{\Gamma(1+i\eta_\nu)}{\Gamma(1-i\eta_\nu)} \frac{e^{-i\eta_\nu \ln \zeta_\nu}}{\zeta_\nu} e^{i\zeta_\nu} [1 + O(\frac{1}{\zeta_\nu})]. \quad (59)$$

Also, in the nonsingular directions for $\nu \neq \alpha$

$$\nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\nu^{(2)}(i\zeta_\nu) = i \nabla_{\mathbf{r}_\alpha} \zeta_\nu + O(1/r_\nu) = i \frac{m_\nu}{m_{\beta\gamma}} k_\nu (\hat{\mathbf{k}}_\nu - \hat{\mathbf{r}}_\nu) + O(1/r_\nu) \quad (60)$$

$$= i \frac{m_\nu}{m_{\beta\gamma}} k_\nu (\hat{\mathbf{k}}_\nu - \epsilon_{\alpha\nu} \hat{\boldsymbol{\rho}}_\alpha) + O(1/\rho_\alpha) \quad (61)$$

and

$$\nabla_{\boldsymbol{\rho}_\alpha} \ln \mathcal{F}_\nu^{(2)}(i\zeta_\nu) = i \nabla_{\boldsymbol{\rho}_\alpha} \zeta_\nu + O(1/r_\nu) = i \epsilon_{\nu\alpha} (-k_\nu \hat{\mathbf{r}}_\nu + \mathbf{k}_\nu) + O(1/r_\nu) \quad (62)$$

$$= i k_\nu (\hat{\boldsymbol{\rho}}_\alpha - \epsilon_{\alpha\nu} \hat{\mathbf{k}}_\nu) + O(1/\rho_\alpha). \quad (63)$$

When deriving (58) we took into account that

$$\left(\frac{1}{2\mu_\nu} \boldsymbol{\Delta}_{\mathbf{r}_\nu} + i \frac{1}{\mu_\nu} \mathbf{k}_\nu \cdot \nabla_{\mathbf{r}_\nu} - V_\nu^C \right) \mathcal{F}_\nu^{(2)}(i\zeta_\nu) = 0. \quad (64)$$

To get an asymptotic equation from Eq. (58) which is valid up to $O(1/\rho_\alpha^3)$, all the coefficients of $O(1)$, $O(1/\rho_\alpha)$ and $O(1/\rho_\alpha^2)$ should be kept in the left-hand-side of the equation. Since in the nonsingular directions in Ω_α region,

$\mathcal{F}_\beta^{(2)}(i\zeta_\beta) \sim O(1/\rho_\alpha)$ only coefficients of $O(1)$ and $O(1/\rho_\alpha)$ in the brackets of Eq. (58) should be left. Taking into account Eqs (44), (61) and (63) we get

$$\begin{aligned} & \left[\frac{1}{2\mu_\alpha} \Delta_{\mathbf{r}_\alpha} + i \frac{1}{\mu_\alpha} \mathbf{k}_\alpha^{(21)}(\boldsymbol{\rho}_\alpha) \cdot \nabla_{\mathbf{r}_\alpha} - V_\alpha(\mathbf{r}_\alpha) \right. \\ & + i \frac{1}{\mu_\alpha} \frac{m_\beta^2}{m_{\beta\gamma}^2} k_\beta \frac{1}{\rho_\alpha} (\mathbf{r}_\alpha - \hat{\boldsymbol{\rho}}_\alpha (\hat{\boldsymbol{\rho}}_\alpha \cdot \mathbf{r}_\alpha)) \cdot \nabla_{\mathbf{r}_\alpha} + i \frac{1}{M_\alpha} \mathbf{q}_\alpha^{(21)} \cdot \nabla_{\boldsymbol{\rho}_\alpha} \\ & \left. - i \epsilon_{\alpha\beta} \frac{1}{m_\alpha} k_\beta (\hat{\mathbf{k}}_\beta - \epsilon_{\alpha\beta} \hat{\boldsymbol{\rho}}_\alpha) \cdot \nabla_{\boldsymbol{\rho}_\alpha} \ln \tilde{\mathcal{F}}_\gamma^{(1)}(i\zeta_{\gamma\alpha}) \right] \varphi_\alpha^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = O(1/\rho_\alpha^2). \end{aligned} \quad (65)$$

Here $\nabla_{\boldsymbol{\rho}_\alpha} \ln \tilde{\mathcal{F}}_\gamma^{(1)}(i\zeta_{\gamma\alpha})$ is given by Eq. (45). We also introduced new local momenta

$$\mathbf{k}_\alpha^{(21)}(\boldsymbol{\rho}_\alpha) = \mathbf{k}_\alpha + \frac{m_\beta}{m_{\beta\gamma}} k_\beta (\hat{\mathbf{k}}_\beta - \epsilon_{\alpha\beta} \hat{\boldsymbol{\rho}}_\alpha) + i(i\eta_\beta + 1) \frac{m_\beta}{m_{\beta\gamma}} \frac{1}{\rho_\alpha} \frac{\hat{\mathbf{k}}_\beta - \epsilon_{\alpha\beta} \hat{\boldsymbol{\rho}}_\alpha}{1 - \epsilon_{\alpha\beta} \hat{\mathbf{k}}_\beta \cdot \hat{\boldsymbol{\rho}}_\alpha}, \quad (66)$$

and

$$\mathbf{q}_\alpha^{(21)}(\boldsymbol{\rho}_\alpha) = \mathbf{q}_\alpha + k_\beta (\hat{\boldsymbol{\rho}}_\alpha - \epsilon_{\alpha\beta} \hat{\mathbf{k}}_\beta). \quad (67)$$

We also took into account that for $\nu \neq \sigma \neq \tau$, $\nu \neq \tau$, $\epsilon_{\nu\tau}$, $\epsilon_{\nu\sigma} = -1$, and

$$-\epsilon_{\alpha\gamma} \frac{1}{m_{\beta\gamma}} (\hat{\mathbf{k}}_\beta - \epsilon_{\alpha\beta} \hat{\boldsymbol{\rho}}_\alpha) + \frac{1}{M_\alpha} (\hat{\boldsymbol{\rho}}_\alpha - \epsilon_{\alpha\beta} \hat{\mathbf{k}}_\beta) = -\epsilon_{\alpha\beta} \frac{1}{m_\alpha} (\hat{\mathbf{k}}_\beta - \epsilon_{\alpha\beta} \hat{\boldsymbol{\rho}}_\alpha). \quad (68)$$

We are looking for a solution of Eq. (66) in the form

$$\varphi_\alpha^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = \varphi_{\alpha(0)}^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) + \frac{\varphi_{\alpha(1)}^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)}{\rho_\alpha}, \quad (69)$$

where $\varphi_{\alpha(0)}^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ satisfies

$$\left[\frac{1}{2\mu_\alpha} \Delta_{\mathbf{r}_\alpha} + i \frac{1}{\mu_\alpha} \mathbf{k}_\alpha^{(21)}(\boldsymbol{\rho}_\alpha) \cdot \nabla_{\mathbf{r}_\alpha} - V_\alpha(\mathbf{r}_\alpha) \right] \varphi_{\alpha(0)}^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = 0. \quad (70)$$

Finally $\varphi_{\alpha(1)}^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) \sim O(1)$ is a solution of equation

$$\begin{aligned} & \left[\frac{1}{2\mu_\alpha} \Delta_{\mathbf{r}_\alpha} + i \frac{1}{\mu_\alpha} \mathbf{k}_\alpha^{(21)}(\boldsymbol{\rho}_\alpha) \cdot \nabla_{\mathbf{r}_\alpha} - V_\alpha(\mathbf{r}_\alpha) \right] \varphi_{\alpha(1)}^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) \\ & = - \left[i \frac{1}{\mu_\alpha} \frac{m_\beta^2}{m_{\beta\gamma}^2} k_\beta (\mathbf{r}_\alpha - \hat{\boldsymbol{\rho}}_\alpha (\hat{\boldsymbol{\rho}}_\alpha \cdot \mathbf{r}_\alpha)) \cdot \nabla_{\mathbf{r}_\alpha} \right] \varphi_{\alpha(0)}^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) \\ & - i \frac{\rho_\alpha}{M_\alpha} \mathbf{q}_\alpha^{(21)} \cdot \nabla_{\boldsymbol{\rho}_\alpha} \varphi_{\alpha(0)}^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) \\ & + i \epsilon_{\alpha\beta} \frac{\rho_\alpha}{m_\alpha} k_\beta (\hat{\mathbf{k}}_\beta - \epsilon_{\alpha\beta} \hat{\boldsymbol{\rho}}_\alpha) \cdot \nabla_{\boldsymbol{\rho}_\alpha} \ln \tilde{\mathcal{F}}_\gamma^{(1)}(i\zeta_{\gamma\alpha}) \varphi_{\alpha(0)}^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha). \end{aligned} \quad (71)$$

Since in Eq. (71) we keep only terms of order $O(1/\rho_\alpha)$ local momentum $\mathbf{k}_\alpha^{(21)}(\boldsymbol{\rho}_\alpha)$ can be replaced by

$$\mathbf{k}_{\alpha(0)}^{(21)}(\boldsymbol{\rho}_\alpha) = \mathbf{k}_\alpha + \frac{m_\beta}{m_{\beta\gamma}} k_\beta (\hat{\mathbf{k}}_\beta - \epsilon_{\alpha\beta} \hat{\boldsymbol{\rho}}_\alpha). \quad (72)$$

A formal solution of Eq. (71) is

$$\begin{aligned} \varphi_{\alpha(1)}^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) & = \varphi_{\alpha(0)}^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) + e^{-\mathbf{k}_{\alpha(0)}^{(21)}(\boldsymbol{\rho}_\alpha) \cdot \mathbf{r}_\alpha} \int d\mathbf{r}'_\alpha G(\mathbf{r}_\alpha, \mathbf{r}'_\alpha) e^{\mathbf{k}_{\alpha(0)}^{(21)}(\boldsymbol{\rho}_\alpha) \cdot \mathbf{r}'_\alpha} \\ & \left[- \left[i \frac{1}{\mu_\alpha} \frac{m_\beta^2}{m_{\beta\gamma}^2} k_\beta (\mathbf{r}'_\alpha - \hat{\boldsymbol{\rho}}_\alpha (\hat{\boldsymbol{\rho}}_\alpha \cdot \mathbf{r}'_\alpha)) \cdot \nabla_{\mathbf{r}_\alpha} \right] \varphi_{\alpha(0)}^{(21)}(\mathbf{r}'_\alpha, \boldsymbol{\rho}_\alpha) \right. \\ & - i \frac{1}{M_\alpha} \mathbf{q}_\alpha^{(21)}(\boldsymbol{\rho}_\alpha) \cdot \nabla_{\boldsymbol{\rho}_\alpha} \varphi_{\alpha(0)}^{(11)}(\mathbf{r}'_\alpha) \\ & \left. - i \epsilon_{\alpha\beta} \frac{1}{m_\alpha} k_\beta (\hat{\mathbf{k}}_\beta - \epsilon_{\alpha\beta} \hat{\boldsymbol{\rho}}_\alpha) \cdot \nabla_{\boldsymbol{\rho}_\alpha} \ln \tilde{\mathcal{F}}_\gamma^{(1)}(i\zeta'_{\gamma\alpha}) \varphi_{\alpha(0)}^{(21)}(\mathbf{r}'_\alpha, \boldsymbol{\rho}_\alpha) \right], \end{aligned} \quad (73)$$

Here $\varphi_{\alpha(0)}^{(21)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ is a solution of the homogeneous Eq. (70).

The third equation for $\varphi_{\alpha(1)}^{(12)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ is obtained by substituting the third term in (38) to (3). Following the same steps, which we used to derive the second equation, or just interchanging $\beta \leftrightarrow \gamma$ in (58) we find $\varphi_{\alpha(1)}^{(12)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ in the following form:

$$\varphi_{\alpha(1)}^{(12)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = \varphi_{\alpha(0)}^{(12)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) + \frac{\varphi_{\alpha(1)}^{(12)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)}{\rho_\alpha}, \quad (74)$$

where $\varphi_{\alpha(0)}^{(12)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ is a solution of

$$\left[\frac{1}{2\mu_\alpha} \Delta_{\mathbf{r}_\alpha} + i \frac{1}{\mu_\alpha} \mathbf{k}_\alpha^{(12)}(\boldsymbol{\rho}_\alpha) \cdot \nabla_{\mathbf{r}_\alpha} - V_\alpha(\mathbf{r}_\alpha) \right] \varphi_{\alpha(0)}^{(12)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = 0. \quad (75)$$

We can derive a similar to Eq. (71) equation for $\varphi_{\alpha(1)}^{(12)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ which has a formal solution

$$\begin{aligned} \varphi_{\alpha(1)}^{(12)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) &= \varphi_{\alpha(0)}^{(12)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) + e^{-\mathbf{k}_\alpha^{(21)}(\boldsymbol{\rho}_\alpha) \cdot \mathbf{r}_\alpha} \int d\mathbf{r}'_\alpha G(\mathbf{r}_\alpha, \mathbf{r}'_\alpha) e^{\mathbf{k}_\alpha^{(12)}(\boldsymbol{\rho}_\alpha) \cdot \mathbf{r}'_\alpha} \\ &\quad [-[i \frac{1}{\mu_\alpha} \frac{m_\beta^2}{m_{\beta\gamma}^2} k_\beta(\mathbf{r}'_\alpha - \hat{\boldsymbol{\rho}}_\alpha(\hat{\boldsymbol{\rho}}_\alpha \cdot \mathbf{r}'_\alpha)) \cdot \nabla_{\mathbf{r}_\alpha}] \varphi_{\alpha(0)}^{(12)}(\mathbf{r}'_\alpha, \boldsymbol{\rho}_\alpha) \\ &\quad - i \frac{1}{M_\alpha} \mathbf{q}_\alpha^{(12)}(\boldsymbol{\rho}_\alpha) \cdot \nabla_{\boldsymbol{\rho}_\alpha} \varphi_{\alpha(0)}^{(11)}(\mathbf{r}'_\alpha) \\ &\quad - i \epsilon_{\alpha\beta} \frac{1}{m_\alpha} k_\beta(\hat{\mathbf{k}}_\beta - \epsilon_{\alpha\beta} \hat{\boldsymbol{\rho}}_\alpha) \cdot \nabla_{\boldsymbol{\rho}_\alpha} \ln \tilde{\mathcal{F}}_\gamma^{(1)}(i\zeta'_\gamma) \varphi_{\alpha(0)}^{(12)}(\mathbf{r}'_\alpha, \boldsymbol{\rho}_\alpha)]. \end{aligned} \quad (76)$$

The fourth equation can be derived after substituting the last term of Eq. (38) into Eq.(3) and it is automatically satisfied up to the terms of order $O(1/\rho_\alpha^3)$ in Ω_α because the product $\mathcal{F}_\beta^{(2)}(i\zeta_\beta) \mathcal{F}_\gamma^{(1)}(i\zeta_\gamma) = O(1/\rho_\alpha^2)$. The fourth term in Eq. (38) leads to an equation for $\varphi_{\alpha(1)}^{(22)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$:

$$\begin{aligned} \mathcal{F}_\beta^{(2)}(i\zeta_\beta) \mathcal{F}_\gamma^{(2)}(i\zeta_\gamma) &\left[\frac{1}{2\mu_\alpha} \Delta_{\mathbf{r}_\alpha} + \frac{1}{2M_\alpha} \Delta_{\boldsymbol{\rho}_\alpha} + i \frac{1}{\mu_\alpha} \mathbf{k}_\alpha \cdot \nabla_{\mathbf{r}_\alpha} + i \frac{1}{M_\alpha} \mathbf{q}_\alpha \cdot \nabla_{\boldsymbol{\rho}_\alpha} \right. \\ &\quad + \frac{1}{\mu_\alpha} [\nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\beta^{(2)}(i\zeta_\beta) + \nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\gamma^{(2)}(i\zeta_\gamma)] \cdot \nabla_{\mathbf{r}_\alpha} \\ &\quad + \frac{1}{M_\alpha} [\nabla_{\boldsymbol{\rho}_\alpha} \ln \mathcal{F}_\beta^{(2)}(i\zeta_\beta) + \nabla_{\boldsymbol{\rho}_\alpha} \ln \mathcal{F}_\gamma^{(2)}(i\zeta_\gamma)] \cdot \nabla_{\boldsymbol{\rho}_\alpha} \\ &\quad \left. - V_\alpha(\mathbf{r}_\alpha) + \frac{1}{\mu_\alpha} \nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\beta^{(2)}(i\zeta_\beta) \cdot \nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\gamma^{(2)}(i\zeta_\gamma) \right. \\ &\quad \left. + \frac{1}{M_\alpha} \nabla_{\boldsymbol{\rho}_\alpha} \ln \mathcal{F}_\beta^{(2)}(i\zeta_\beta) \cdot \nabla_{\boldsymbol{\rho}_\alpha} \ln \mathcal{F}_\gamma^{(2)}(i\zeta_\gamma) \right] \times \varphi_{\alpha(1)}^{(22)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = O(1/\rho_\alpha^3). \end{aligned} \quad (77)$$

Using the same arguments we have used before, we may drop all the terms containing derivatives over ρ_α when looking for a solution in leading order. Then the equation for $\varphi_{\alpha(1)}^{(22)}$ reduces to

$$\left[\frac{1}{2\mu_\alpha} \Delta_{\mathbf{r}_\alpha} + i \frac{1}{\mu_\alpha} \mathbf{k}_\alpha^{(22)}(\boldsymbol{\rho}_\alpha) \cdot \nabla_{\mathbf{r}_\alpha} - V_\alpha(\mathbf{r}_\alpha) \right] \varphi_{\alpha(1)}^{(22)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = 0, \quad (78)$$

with a local momentum

$$\mathbf{k}_\alpha^{(22)}(\boldsymbol{\rho}_\alpha) = \mathbf{k}_\alpha + \sum_{\nu=\beta,\gamma} \frac{m_\nu}{m_{\beta\gamma}} k_\nu (\hat{\mathbf{k}}_\nu - \epsilon_{\alpha\nu} \hat{\boldsymbol{\rho}}_\alpha). \quad (79)$$

If V_α is a pure Coulomb potential, $V_\alpha = V_\alpha^C$, then Eqs (55), (70), (75), (78) have the following solution

$$\varphi_{\alpha(1)}^{(ij)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = N_\alpha^{(ij)}(\boldsymbol{\rho}_\alpha) F(-i\eta_\alpha^{(ij)}(\boldsymbol{\rho}_\alpha), 1; i\zeta_\alpha^{(ij)}(\boldsymbol{\rho}_\alpha)), \quad (80)$$

Here, $i = 1, 2; j = 1, 2$ and $N_\alpha^{(ij)}(\boldsymbol{\rho}_\alpha)$ is defined as

$$N_\alpha^{(ij)}(\boldsymbol{\rho}_\alpha) = e^{-\pi\eta_\alpha^{(ij)}(\boldsymbol{\rho}_\alpha)/2} \Gamma(1 + i\eta_\alpha^{(ij)}(\boldsymbol{\rho}_\alpha)), \quad (81)$$

where $\eta_{\alpha}^{(ij)}(\boldsymbol{\rho}_{\alpha}) = \frac{z_{\beta}z_{\gamma}e^2\mu_{\alpha}}{k_{\alpha}^{(ij)}(\boldsymbol{\rho}_{\alpha})}$, and $\zeta^{(ij)}(\boldsymbol{\rho}_{\alpha}) = k_{\alpha}^{(ij)}(\boldsymbol{\rho}_{\alpha})r_{\alpha} - \mathbf{k}_{\alpha}^{(ij)}(\boldsymbol{\rho}_{\alpha}) \cdot \mathbf{r}_{\alpha}$.

If V_{α} is not a pure Coulomb potential, then the differential equations above, which parametrically depend on $\boldsymbol{\rho}_{\alpha}$, should be solved numerically. Since all equations are of the two-body type, numerical methods are well developed and have been in use for a long time. They can be applied to solve the differential equations above as well. All the solutions found this way are valid in all directions of the asymptotic region Ω_{α} except for singular directions.

Thus, returning to Eq. (38) we can claim that, having derived all four wave functions $\varphi_{\alpha(1)}^{(ij)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$, $i, j = 1, 2$, we know the asymptotic behavior of the three-body incident wave of the scattering wave function of the first type in the asymptotic region Ω_{α} up to terms $O(1/\rho_{\alpha}^3)$.

V. GENERALIZED ASYMPTOTIC SCATTERING WAVE FUNCTION VALID IN ALL REGIONS Ω_{ν} , $\nu = \alpha, \beta, \gamma$

Now we are in position to present a generalized asymptotic scattering wave function which satisfies the Schrödinger equation up to second order and which is valid in all the asymptotic regions:

$$\Psi_{\mathbf{k}_{\alpha}\mathbf{q}_{\alpha}}^{(\alpha\beta\gamma)(+)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha}) \equiv e^{i\mathbf{k}_{\alpha} \cdot \mathbf{r}_{\alpha} + i\mathbf{q}_{\alpha} \cdot \boldsymbol{\rho}_{\alpha}} \varphi_{\mathbf{k}_{\alpha}}^{\sim}(\mathbf{r}_{\alpha}) \varphi_{\mathbf{k}_{\beta}}^{\sim}(\mathbf{r}_{\beta}) \varphi_{\mathbf{k}_{\gamma}}^{\sim}(\mathbf{r}_{\gamma}). \quad (82)$$

After substituting (82) into (3) and dropping the higher order terms we get,

$$\begin{aligned} & \{E - T_{\mathbf{r}_{\alpha}} - T_{\tilde{\rho}_{\alpha}} - V\} [e^{i\mathbf{k}_{\alpha} \cdot \tilde{\mathbf{r}}_{\alpha} + i\mathbf{q}_{\alpha} \cdot \boldsymbol{\rho}_{\alpha}} \varphi_{\mathbf{k}_{\alpha}}^{\sim}(\mathbf{r}_{\alpha}) \varphi_{\mathbf{k}_{\beta}}^{\sim}(\mathbf{r}_{\beta}) \varphi_{\mathbf{k}_{\gamma}}^{\sim}(\mathbf{r}_{\gamma})] \\ &= e^{i\mathbf{k}_{\alpha} \cdot \mathbf{r}_{\alpha} + i\mathbf{q}_{\alpha} \cdot \boldsymbol{\rho}_{\alpha}} \varphi_{\mathbf{k}_{\alpha}}^{\sim}(\mathbf{r}_{\alpha}) \varphi_{\mathbf{k}_{\gamma}}^{\sim}(\mathbf{r}_{\gamma}) \left[\frac{\Delta_{\mathbf{r}_{\alpha}}}{2\mu_{\alpha}} + \frac{i\tilde{\mathbf{k}}_{\alpha} \cdot \nabla_{\mathbf{r}_{\alpha}}}{\mu_{\alpha}} - V_{\alpha} \right] \varphi_{\mathbf{k}_{\alpha}}^{\sim}(\mathbf{r}_{\alpha}) \\ &+ e^{i\mathbf{k}_{\beta} \cdot \mathbf{r}_{\beta} + i\mathbf{q}_{\beta} \cdot \boldsymbol{\rho}_{\beta}} \varphi_{\mathbf{k}_{\alpha}}^{\sim}(\mathbf{r}_{\alpha}) \varphi_{\mathbf{k}_{\gamma}}^{\sim}(\mathbf{r}_{\gamma}) \left[\frac{\Delta_{\mathbf{r}_{\beta}}}{2\mu_{\beta}} + \frac{i\tilde{\mathbf{k}}_{\beta} \cdot \nabla_{\mathbf{r}_{\beta}}}{\mu_{\beta}} - V_{\beta} \right] \varphi_{\mathbf{k}_{\beta}}^{\sim}(\mathbf{r}_{\beta}) \\ &+ e^{i\mathbf{k}_{\gamma} \cdot \mathbf{r}_{\gamma} + i\mathbf{q}_{\gamma} \cdot \boldsymbol{\rho}_{\gamma}} \varphi_{\mathbf{k}_{\alpha}}^{\sim}(\mathbf{r}_{\alpha}) \varphi_{\mathbf{k}_{\beta}}^{\sim}(\mathbf{r}_{\beta}) \left[\frac{\Delta_{\mathbf{r}_{\gamma}}}{2\mu_{\gamma}} + \frac{i\tilde{\mathbf{k}}_{\gamma} \cdot \nabla_{\mathbf{r}_{\gamma}}}{\mu_{\gamma}} - V_{\gamma} \right] \varphi_{\mathbf{k}_{\gamma}}^{\sim}(\mathbf{r}_{\gamma}) \\ &= \begin{cases} O(\frac{1}{r_{\alpha}^2}, \frac{1}{r_{\beta}^2}, \frac{1}{r_{\gamma}^2}), \mathbf{r}_{\alpha}, \mathbf{r}_{\beta}, \mathbf{r}_{\gamma} \in \Omega_0 \\ O(\frac{1}{r_{\beta}^2}, \frac{1}{r_{\gamma}^2}), \mathbf{r}_{\beta}, \mathbf{r}_{\gamma} \in \Omega_{\alpha} \\ O(\frac{1}{r_{\alpha}^2}, \frac{1}{r_{\gamma}^2}), \mathbf{r}_{\alpha}, \mathbf{r}_{\gamma} \in \Omega_{\beta} \\ O(\frac{1}{r_{\alpha}^2}, \frac{1}{r_{\beta}^2}), \mathbf{r}_{\alpha}, \mathbf{r}_{\beta} \in \Omega_{\gamma} \end{cases}, \end{aligned} \quad (84)$$

where the local momentum is given by

$$\tilde{\mathbf{k}}_{\nu} = \mathbf{k}_{\nu} - i \sum_{\tau=\alpha, \beta, \gamma} (1 - \delta_{\nu, \tau}) \nabla_{\mathbf{r}_{\nu}} \ln \varphi_{\mathbf{k}_{\tau}}^{\sim}. \quad (85)$$

In the asymptotic region Ω_0 , each local momentum, $\tilde{\mathbf{k}}_{\nu}$, can be replaced by the corresponding asymptotic momentum, \mathbf{k}_{ν} . In the asymptotic region Ω_{α} , Eq.(84) reduces to the one quasi-two-particle differential equations:

$$\left[\frac{\Delta_{\mathbf{r}_{\alpha}}}{2\mu_{\alpha}} + \frac{i\tilde{\mathbf{k}}_{\alpha} \cdot \nabla_{\mathbf{r}_{\alpha}}}{\mu_{\alpha}} - V_{\alpha} \right] \varphi_{\mathbf{k}_{\alpha}}^{\sim}(\mathbf{r}_{\alpha}) = O(\frac{1}{r_{\beta}}, \frac{1}{r_{\gamma}}). \quad (86)$$

Solution of this equation is evident and provides the Coulomb-nuclear scattering wave function with the local momentum $\tilde{\mathbf{k}}_{\alpha}$. Similarly we can get the asymptotic solution in leading order in the other two asymptotic regions Ω_{β} and Ω_{γ} .

VI. CONCLUSION

We derived the three-body asymptotic incident wave, which satisfies the Schrödinger equation in the asymptotic region Ω_{ν} , $\nu = \alpha, \beta, \gamma$ up to terms of order $1/\rho_{\nu}^3$. This asymptotic incident wave gives the leading asymptotic terms of the three-body scattering wave function of the first type and is an extension of the asymptotic wave function derived in [2, 3]. Equivalently, similar wave functions satisfy the Schrödinger equation up to $O(1/\rho_{\nu}^3)$, $\nu = \beta, \gamma$. It is worth

mentioning that the asymptotic solution satisfying the Schrödinger equation, in the asymptotic region Ω_ν up to the $O(1/\rho_\nu^2)$ can be found analytically [2, 3]. To find an asymptotic solution satisfying the Schrödinger equation in Ω_ν up to terms of $O(1/\rho_\nu^3)$ we need to solve two-body type differential equations numerically. The next order term in the asymptotic three-body scattering wave function represents the outgoing $3 \text{ particles} \rightarrow 3 \text{ particles}$ scattered wave and has been given in [7].

The resulting asymptotic solution provides extended boundary conditions in all the asymptotic regions and can be used in the direct numerical solution of the Schrödinger equation or in approximate perturbation calculations as a leading asymptotic term of the three-body scattering wave function.

Acknowledgments

This work was supported by the U. S. DOE under Grant No. DE-FG03-93ER40773, by NSF Award No. PHY-0140343 and the Australian Research Council.

-
- [1] L. D. Faddeev and S. P. Merkuriev, *Quantum Scattering Theory for Several Particle Systems* (Kluwer Academic Publishers, Dordrecht, 1993).
 - [2] E. O. Alt and A. M. Mukhamedzhanov, Phys. Rev. A **47**, 2004 (1993).
 - [3] A. M. Mukhamedzhanov and M. Lieber, Phys. Rev. A **54**, 3078 (1996).
 - [4] A. S. Kadyrov, A. M. Mukhamedzhanov, and A. T. Stelbovics, Phys. Rev. A **67**, 024702 (2003).
 - [5] A. S. Kadyrov, A. M. Mukhamedzhanov, A. T. Stelbovics, I. Bray, and F. Pirlepesov, Phys. Rev. A **68**, 022703 (2003).
 - [6] A. S. Kadyrov, A. M. Mukhamedzhanov, A. T. Stelbovics, and I. Bray, Phys. Rev. Lett. **91**, 253202 (2003).
 - [7] A. S. Kadyrov, A. M. Mukhamedzhanov, A. T. Stelbovics, and I. Bray, Phys. Rev. A **70**, 062703 (2004).
 - [8] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics (Non-relativistic theory)*, vol. 3 of *Course of theoretical physics* (Pergamon press, Oxford, 1985), 3rd ed.
 - [9] A. Kratzer and W. Franz, *Transzendente Funktionen* (Akadem. Verlagsgesellschaft, Leipzig, 1963), 2nd ed.
 - [10] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series and Products* (Academic Press, San Diego, 1980).
 - [11] P. J. Redmond, described in [12] (unpublished).
 - [12] L. Rosenberg, Phys. Rev. D **8**, 1833 (1973).
 - [13] C. R. Garibotti and J. E. Miraglia, Phys. Rev. A **21**, 572 (1980).